The 5th
PAL-XFEL
Users' Meeting

July 2-3, 2025

POSCO International Center, POSTECH

http:s//pal.postech.ac.kr/2025palxfelum

Invited Speakers

Bumjoon Kim (POSTECH)
Dongbin Shin (GIST)
Joonseok Lee (Hanyang University)
Tae Kyu Kim (KAIST)
Wonchull Kang (Soongsil University)

PAL POHANG ACCELERATOR LABORATORY

KOSUA 한국방사광이용자협회
The Korean Synchrotron Radiation User's Association

Ministry of Science and ICT

The 5th PAL-XFEL Users' Meeting

PAL-XFEL
JULY 2~3, 2025

주최 : 포항가속기연구소
주관 : (사)한국방사광이용자협회
후원 : 과학기술정보통신부

The 5th PAL-XFEL Users' Meeting

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No.	번 호	발표자	소 속	초 록 제 목
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2	IT-02	이준석	한양대학교	In situ study of photocatalytic strain evolution and charge transfer in a single metal nanoparticle
3	IT-03	강원철	숭실대학교	Capturing the Catalytic Cycle of Cysteine Desulfurase: Structural Snapshots of Active and Inhibited States
4	IT-04	김태규	KAIST	Photochemistry of the Biologically Relevant Disulfide Molecules by Femtosecond X-ray Spectroscopy
5	IT-05	신동빈	GIST	Light-induced ultrafast dynamics in 2D layered system
6	ST-01	이성윤(송창용)	POSTECH	Deep learning for coherent diffraction imaging using XFEL
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8	PS-01	장호영, 천세환	PAL	Ultrafast Photo-induced Dynamics in Condensed Matter at PAL-XFEL
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10	PS-03	이상재	PAL	Advancing Toward a Successful SFX Experiment and Data Processing
11	PS-04	김수남, 박상한	PAL	Discussion on Imaging Science in PAL-XFEL
12	PP-01	구자인(이효철)	KAIST/IBS	Ultrafast structural dynamics of I_2 in methanol visualized with femtosecond X-ray liquidography
13	PP-02	이성용(박재훈)	POSTECH	Time-domain decoding of unconventional charge order mechanisms in nonmagnetic and magnetic kagome metals
14	PP-03	남경민(김경환)	POSTECH	Investigating electrospray with X-ray Scattering
15	PP-04	고세리(강원철)	숭실대학교	Crystal structure of dicarboxylate-mediated inhibition of cysteine desulfurase
16	PP-05	우태균(김태규)	KAIST	Unveiling Photo-excited Electron Trapping Dynamics at Self-Reduced TiO_2 via Time-Resolved X-ray Absorption Spectroscopy
17	PP-06	윤규석(김현정)	서강대학교	The correlation between crystal defect and plasma induced by femtosecond laser in crystalline Cu thin-films
18	PP-07	이은수(강원철)	숭실대학교	Crystallographic Snapshots of an ATP-bound Human p97 N-D1 Hexamer using X-ray Free-Electron Lasers
19	PP-08	김신우(송창용)	POSTECH	Void evolution in ultrafast melting of Au nanoparticles driven by light's angular momentum using time-resolved imaging at XFEL
20	PP-09	이준호(김태규)	KAIST	Tracking Ligand Charge Delocalization Mediated Charge transfer dynamics of Bridged bimetallic complex
21	PP-10	김우혁(김태우)	경희대학교	Development of Femtosecond X-ray Emission Spectrometer Based on von Hamos geometry
22	PP-11	오세현(강민구)	서울대학교	Evidence of a light-induced metastable state in charge-ordered 4*d*-kagome metals

Abstracts of Invited Talk

[IT-01]

Liquid-like spin dynamics in square-lattice iridates

Bumjoon Kim

Department of Physics, Pohang University of Science and Technology,
Pohang 37673, Korea,

Spinons are fractional spin excitation that are of great interest in condensed matter physics due to their connection to superconductivity and topological orders. Although their existence in two diemensions remain controversial, an anomalous feature ubiquitous in the excitation spectrum of squre-lattice cuprates, known as ‘(π,0) anomaly’ has been interpreted as a spin continuum. The pseudospin-1/2 Heisenberg antiferromaget realized in square-lattice iridates can provide a fresh new insight into this long-standing issue, as they can be studied using hard x-ray resonant inelastic x-ray scattering (RIXS) over a wide momentum region. In thi talk, I will talk about our recent results on sqaure-lattice iridates. By measuring the spectra in different scattering geometries, we are able to resolve transverse and longitudinal channels, and thereby separate the singe-magnon component and the continuum. Our result shows that the (π,0) anomaly spectrum of single-layer Sr_2IrO_4 is fully isotropic, implying complete breakdown of magnons, This result provides strong evidence for the existence of spinons in the square-lattice iridates. Surprisingly, such behavior is found in the entire region along the zone boundary when in a superlattice that has alternating stacking of single and double layers. Using time-resolved resonant x-ray diffraction, we find that this enhanced frustration manifests as longer timescale for recovery of the magnetic order after it has been transiently suppressed by an optical pump laser pulse. Our results show that recovery dyamics probed by ultrafast x-ray can be a novel route to study frustrated magnetism.

[IT-02]

In situ study of photocatalytic strain evolution and charge transfer in a single metal nanoparticle

S. H. Park*, S. Kim*, S. Kim*, W. Cha**, J. Lee*

*Department of Chemistry, Hanyang University, Seoul 04763, Korea,
**X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

Photocatalysis is a promising technique due to its capacity to efficiently harvest solar energy and its potential to address the global energy crisis. However, the structure⁻activity relationships of photocatalyst during wavelength-dependent photocatalytic reactions remains largely unexplored because it is difficult to measure under operating conditions. Here we show the photocatalytic strain evolution of a single Au nanoparticle (AuNP) supported on a TiO_2 film by combining three-dimensional (3D) Bragg coherent X-ray diffraction imaging with an external light source. The wavelength-dependent generation of reactive oxygen species (ROS) has significant effects on the structural deformation of the AuNP, leading to its strain evolution. Density functional theory (DFT) calculations are employed to rationalize the induced strain caused by the adsorption of ROS on the AuNP surface. These observations provide insights of how the photocatalytic activity impacts on the structural deformation of AuNP, contributing to the general understanding of the atomic-level catalytic adsorption process.

[IT-03]

Capturing the Catalytic Cycle of Cysteine Desulfurase: Structural Snapshots of Active and Inhibited States

Wonchull Kang

Department of Chemistry, Soongsil University, Seoul 06978, Korea

Iron-sulfur (Fe-S) clusters are indispensable cofactors for a wide array of metabolic enzymes involved in respiration, nitrogen fixation, DNA repair, and redox regulation. The biosynthesis of Fe-S clusters is tightly coordinated with cellular metabolic states. Cysteine desulfurases, such as IscS, SufS, and NifS, initiate Fe-S cluster formation by catalyzing sulfur transfer from cysteine to downstream scaffold proteins. Despite their central roles, structural insights into their catalytic intermediates remain limited. We investigated the catalytic mechanisms of *Azotobacter vinelandii* NifS using serial femtosecond crystallography at PAL-XFEL. To capture the transient intermediates of the catalytic cycle, we utilized a photocaged cysteine that enabled time-resolved structural studies of the enzymatic reaction. By triggering catalysis with a laser pulse and collecting diffraction data 1 µs post-activation, we obtained a structure that represented the early substrate-bound state. This structure reveals a previously unresolved conformation of the catalytic loop, suggesting that it plays a key role in substrate positioning and potentially in persulfide transfer during catalysis. In parallel, we solved the inhibitor-bound structures of NifS in complex with the dicarboxylate metabolites malonate and succinate. Strikingly, both metabolites occupy the canonical cysteine-binding site, and sterically preventing substrate access. Enzymatic assays revealed that the dicarboxylate inhibitor reduced activity by approximately 10%. These results suggest that even modest inhibition by dicarboxylates may reflect a direct and previously unrecognized regulatory link between TCA cycle flux and Fe-S cluster biogenesis. Together, theses structural snapshots provide a high-resolution view of NifS in both its active and inhibited states, and support a model in which Fe-S cluster biogenesis is finely tuned by the metabolic environment. This work lays the groundwork for understanding how cells integrate nutrient state with essential cofactor production at the molecular level.

[IT-04]

Photochemistry of the Biologically Relevant Disulfide Molecules by Femtosecond X-ray Spectroscopy

T. K. Kim

Department of Chemistry, Korea Advanced Insitute of Science and
Technology (KAIST), Daejeon 34141, Korea

The disulfide bond is one of the most important structure-making moieties in proteins, stabilizing the latter's tertiary structure when two spatially adjacent L-cystinyl form a covalent disulfide bond - the disulfide bridge. In aliphatic disulfides, the emergence of several photoproducts after UV irradiation has been reported over the past five decades, the formation mechanism and yields of which are still controversial. Time-resolved X-ray absorption spectroscopy (TR-XAS) is uniquely positioned to identify with high chemical specificity the nature of the earliest photoproducts by probing the sulfur core-level transitions. We have demonstrated that TR-XAS at the S K-edge is a chemically sensitive tool to observe the UV photochemistry of small organosulfur compounds in nonpolar solvents. We investigated the natural amino acid dimer L-cystine in aqueous solution and also performed the same experiments in a tripeptide dimer bound by a disulfide bridge (glutathione disulfide, GSSG) in a bottom-up approach to find that L-cystine already captures the essence of the ultrafast photochemistry of the disulfide bridge in aliphatic disulfides. We conclude that upon 267 nm irradiation, aliphatic disulfides in aqueous solution immediately and exclusively undergo homolytic bond cleavage leading to the formation of two identical radicals. The subsequent geminate recombination of the thiyl radicals at ~3eV above the L-cystine ground state occurs with a time constant of ~600 fs, resulting in the formation of a secondary product on the L-cystine ground-state potential energy surface. We attribute the secondary reaction to perthiyl radical generation, a process only possible in condensed phases. We believe that we have conclusive evidence to the long-debated perthiyl radical generation mechanism from the first application of femtosecond XAS in the tender X ray regime (2 - 5 keV) to organic photochemistry in solution.

[IT-05]

Light-induced ultrafast dynamics in 2D layered system

D. Shin

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Condensed-matter systems have attracted significant interest due to their intriguing physical properties and potential applications. Recent studies have revealed that light can profoundly modify material properties, leading to unprecedented light-induced phenomena. Notably, experiments have demonstrated light-induced topological phase transitions in the layered material WTe_2. These transitions are driven by lattice distortions originating from excited electronic states in WTe_2. In this talk, I will present theoretical studies of light-induced dynamics in other layered systems, specifically trilayer WSe_2 and MXene. Through the displacive excitation of coherent phonons, we demonstrate two unique phenomena: (1) light-controlled interlayer spacing in trilayer WSe_2, and (2) light-driven ultrafast carrier dynamics in MXene. These studies provide insight into the microscopic mechanisms whereby light induces ultrafast structural and electronic dynamics in layered condensed-matter systems.

Abstracts of Student Talk

[ST-01]

Deep learning for coherent diffraction imaging using XFEL

S. Y. Lee, C. Song

Department of Physics and Photon Science Center, Pohang University of Science and Technology, Pohang 37673, Republic of Korea, Center for Ultrafast Science on Quantum Matter, Max Planck POSTECH/Korea Research Initiative, Pohang 37673, Republic of Korea.

Coherent diffraction imaging has enabled high-resolution diffraction-limited imaging of various specimens, fully utilizing advantages of short-wavelength sources regardless of performance of imaging optics. Time-resolved imaging has also been realized by single-pulse measurements using XFEL, offering nm-sub-ps spatiotemporal resolution that enables to track ultrafast dynamics of nanoscale structures. However, despite such superiority, strong noise and partial occlusion of diffraction data from XFEL experiments demand complicated data processing with meticulous human inspection, and these become severe with excessive amounts of data measured during the experiments. In this circumstance, deep learning can be a solution to handle such pouring data. In this talk, our efforts on developing deep-learning models for real-space image reconstruction from noisy, imperfect diffraction data will be introduced. Dedicated neural network architectures and data generation strategies were proposed, reflecting characteristics of diffraction signals and maximally minimizing human and physical biases, and they were demonstrated their remarkable performance along with general applicability and rapid processing time. Our approaches will be a worthy platform for applying deep learning to X-ray diffraction data, enabling real-time data processing for upcoming high-repetition-rate X-ray sources.

[ST-02]

Tracking the Melting Dynamics of Crystalline Ice using Time-resolved X-ray Scattering at PAL-XFEL

K. Park*, K. H. Kim*

*Department of Chemistry, Pohang University of Science and Technology,
Pohang, 790-784, Kyungbuk, Korea

The melting of ice and the recrystallization of liquid water have been extensively studied due to the fundamental importance of water as one of the abundant and vital substances for life on Earth. However, despite the numerous studies using time-resolved optical spectroscopies and molecular dynamics simulation, the detailed mechanisms of ice melting in terms of structural dynamics have not been fully elucidated. In this study, we employed a rapid temperature jump in conjunction with an intense X-ray pulse from free-electron lasers (FELs) as a probe to elucidate the detailed structural dynamics of ice melting. To investigate the melting and recrystallization dynamics of crystalline ice I, we conducted a time-resolved X-ray scattering experiment in the time window from ns to µs. Using information extracted from the wide-angle X-ray scattering (WAXS) and small-angle X-ray scattering (SAXS) patterns, we estimated the time-dependent changes in the size and number of liquid domains, indicating that partial melting and superheating of ice occurs at around 20 ns. More recently, we extended the time window to cover ps to µs and observed interesting melting features on both the ps and ns timescales through detailed analysis of the time-resolved SAXS and WAXS data.

Abstracts of Parallel Session

[PS-01]

Parallel Session: Ultrafast Photo-induced Dynamics in Condensed Matter at PAL-XFEL

Convener : Hoyoung Jang and Sae Hwan Chun

In this session, we intend to bring together researchers studying ultrafast photo-induced dynamics in condensed matter. This session will highlight the scientific opportunities available at PAL-XFEL, review the current status of experimental facilities, and gather insights through user feedback.

Agenda

Time	Ultrafast Photo-Induced Dynamics in Condensed Matter: Research Topics by Ph.D. Students	
16:10-16:30	Frustrated phonon with charge density wave (CDW) in vanadium Kagome metal	Seung-Phil Heo (POSTECH)
16:30-16:50	Nematic response of FeTe in the ultrafast dynamics	Jihyeon Hwang (Chungbuk National Univ.)
16:50-17:00	Break	
	Ultrafast Photo-Induced Dynamics in Condensed Matter: Brief Reviews of Experimental Capabilities at PAL	
17:00-17:20	fs-THz beamline at PLS-II	Hee Jun Shin (PAL)
17:20-17:35	Femtosecond X-ray Scattering (FXS) at PAL-XFEL	Sae Hwan Chun (PAL)
17:35-17:50	Resonant soft X-ray Scattering (RSXS) at PAL-XFEL	Hoyoung Jang (PAL)
17:50-18:10	Open discussion and feedback	Everyone

[PS-02]

Parallel Session: Exploring Chemical Reaction Dynamics with PAL-XFEL : A Symposium for Young Scientists

Convener : Jae Hyuk Lee and Sang Han Park

We're very excited to bring together young scientists working on ultrafast chemical reaction dynamics. We'll take a look at the current state of experimental setups at PAL-XFEL, such as time-resolved X-ray spectroscopy and time-resolved X-ray liquidography, and discuss ongoing research.

Agenda

Time	**Exploring Chemical Reaction Dynamics with PAL-XFEL :** **A Symposium for Young Scientists**	
16:10-16:35	Polaron study via Density Functional Theory calculation.	Kwangsik Jeong (Yonsei Univ.)
16:35-17:00	Wavelength-Dependent Structural Dynamics of $[Au(CN)_2^-]_3$ Studied by Time-Resolved X-ray Liquidography	Hosung Ki (IBS)
17:00-17:10	Break	
17:10-17:30	Dynamics of Photo-excited Charge Carriers in Liquid phase α-TiO_2 measured using ultrafast tr-XAS	Abhishek Katoch (Yonsei Univ.)
17:30-17:50	Solvent-dependent isomer formation dynamics of iodoform investigated via X-ray liquidography at PAL-XFEL	Yongjun Cha (KAIST)
17:50-18:10	Elucidating Photoinduced Dynamics of Thioketone Molecules	Haneol Oh (KAIST)

[PS-03]

Parallel Session: Advancing Toward a Successful SFX Experiment and Data Processing

Convener : Sang Jae Lee

In this session, we aim to clearly and simply explain the process of studying protein structures - from sample preparation to data collection using the SFX (Serial Femtosecond Crystallography) technique, and finally data analysis. We will also have a Q&A and discussion session to address any questions or topics of interest.

Agenda

Time	Advancing Toward a Successful SFX Experiment and Data Processing
16:10-16:30	Sample preparation to acquire microcrystals using batch mode (inc. alternative way)
16:30-16:50	SFX Experiment
16:50-17:00	Data Preprocessing
17:00-17:30	Data Calculation, checking statistics
17:30-17:40	From obtaining a structure factor file to solve a protein structure
17:40-17:50	Case study
17:50-18:10	Open discussion and feedback

[PS-04]

Parallel Session: Discussion on Imaging Science in PAL-XFEL

Convener : Sunam Kim and Sang Han Park

We're glad to bring together researchers interested in ultrafast imaging science. In this parallel session, we are going to discuss the current states of ultrafast imaging science in PAL-XFEL including time resolved -Fourier Transform Holography (tr-FTH), -Bragg Coherent X-ray Diffraction Imaging(tr-BCDI), and so on.

Agenda

Time	**Ultrafast Imaging Science**	
16:10-16:35	Light⁻Induced Ultrafast X-Ray Imaging via Fourier Transform Holography (FTH)	Dr. Sang Han Park (PAL-XFEL)
16:35-17:00	Femtosecond Time Resolved Bragg Coherent Diffraction Imaging (tr-BCDI)	Dr. Sunam Kim (PAL-XFEL)
17:00-17:10	Break	
17:10-17:35	Time-resolved single-particle imaging at XFEL facility	Dr. Chan Kim (European XFEL)
17:35-18:10	Open Discussion	

Abstracts of Poster Presentation

[PP-01]

Ultrafast structural dynamics of I_2 in methanol visualized with femtosecond X-ray liquidography

J. Gu, J. H. Lee*, H. Ihee**

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Understanding solute–solvent interactions on the femtosecond timescale is essential for elucidating the mechanisms that govern chemical reactions in solution. Yet, directly observing these interactions at atomic resolution remains a major challenge. In this study, we investigated the photodissociation of molecular iodine (I2) in methanol using femtosecond time-resolved X-ray liquidography (fs-TRXL). Upon 400 nm photoexcitation, I2 bifurcates into two excited-state intermediates with abnormally extended I–I bond lengths (4.88 Å and 3.97 Å), both forming within 500 fs and decaying on different timescales. Quantum chemical calculations reveal that these species are only stabilized when methanol molecules are treated explicitly, confirming that direct solute–solvent coordination is essential for their formation. Furthermore, fs-TRXL captures coherent vibrational motion of the solute and ultrafast reorganization of the surrounding solvent shell, showing that the solvent cage dynamically expands with I–I bond elongation. These results provide direct structural evidence that solute–solvent interactions actively reshape the reaction coordinate from its earliest stage, emphasizing their crucial role in modulating photochemical pathways in solution.

[PP-02]

Time-domain decoding of unconventional charge order mechanisms in nonmagnetic and magnetic kagome metals

S. Lee[1,2], B. Lee[1,2], H. Jang[3], X. Wu[4], J. Kim[1,2], G. Kang[3], C. Won[1,5],
H. Choi[3], S. Y. Park[6], K. M. Shen[7,8], F. Cilento[9], A. Wang[4],
J. H. Park[1,2] & M. Kang[1,7,8,10]

[1]cCMR, MPK, Pohang 37673, Korea. [2]Dept. of Physics, POSTECH, Pohang 37673, Korea. [3]PAL-XFEL, Pohang 37673, Korea. [4]College of Physics and Center of Quantum Materials and Devices, Chongqing University, Chongqing 401331, China. [5]IPEM, Pohang 37673, Korea. [6]PAL, Pohang 37673, Korea. [7]LASSP, Dept. of Physics, Cornell University, Ithaca, New York 14853, USA. [8]Kavli Institute at Cornell for Nanoscale Science, Cornell University, Ithaca, New York 14853, USA. [9]Elettra−Sincrotrone Trieste S.C.p.A., S. S. 14, km 163.5 in AREA Science Park, Trieste 34149, Italy. [10]Dept. of Physics and Astronomy, SNU, Seoul 08826, Korea.

Kagome lattice materials have been actively studied in recent years due to their potential to host exotic orders such as superconductivity, magnetism, and charge order. However, static measurements alone have not been sufficient to clearly reveal the exact nature of these orders, leaving many aspects unresolved. In this work, at an X-ray free-electron laser, we performed time-resolved X-ray diffraction studies on two charge-ordered Kagome lattice materials— nonmagnetic ScV6Sn6 and magnetic FeGe—to identify the dominant order parameter governing their ultrafast dynamics over the time-axis.

In nonmagnetic ScV6Sn6, we observed ultrafast melting and an amplitude mode, signatures of the electron-phonon coupled charge order. In contrast, magnetic FeGe exhibited resilient metastable dynamics, originating from its unique magnetism-interlocked charge order. Our results not only provide fundamental insight into charge order formation but also pave the way for future out-of-equilibrium engineering of novel quantum orders in this versatile lattice platform.

[PP-03]

Investigating electrospray with X-ray Scattering

K. Nam, M. Hwang, M. Kim, J. Seo*, K. H. Kim*
Department of Chemistry, Pohang University of Science and Technology,
Pohang, 790-784, Kyungbuk, Korea

Electrospray ionization (ESI) is a method to make a solution sample into gaseous ions by inducing Coulombic explosion of the sample droplets under strong electric field. While the droplets are getting smaller, unique molecular behaviors different from those in bulk solution appear such as acceleration of the reactions. However, since the nanodroplets are tiny, the detailed mechanism of these intriguing properties is not explored clearly so far. Here, we utilized ultra-short and super-bright X-ray pulse from X-ray free electron laser (XFEL), which enables us to observe samples of molecular-scales. We successfully estimate the sizes of the nanodroplets by analyzing Airy pattern from SAXS, and by using nanofocused X-ray beam, we could find traces from solute molecules and extract concentration of each shot from WAXS.

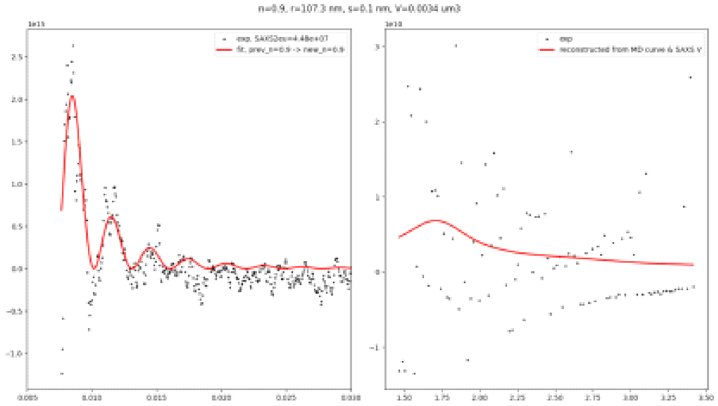

Figure 1 Estimated size of the nanodroplet (n=0.9, r±σ=107.3±0.1 nm)

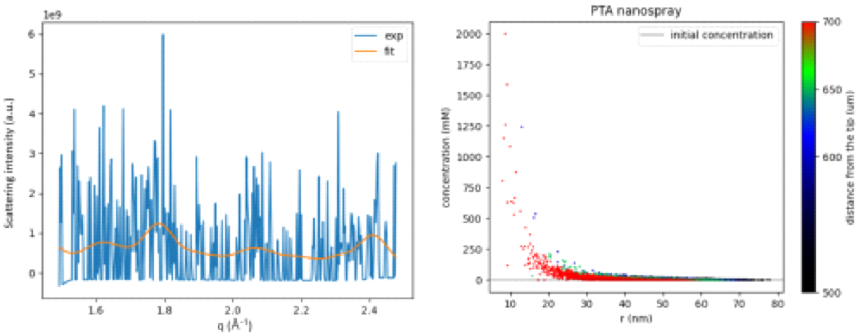

Figure 2 single-shot basis fit result (left), and ensemble behavior (right)

[PP-04]

Crystal structure of dicarboxylate-mediated inhibition of cysteine desulfurase

Seri Koh, Yeeun Kim, Eunsoo Lee, Rang Choi, Suah Cho, Sooyeon Jeong, Wonchull Kang

Department of Chemistry, Soongsil University, Seoul 06978, Korea

Iron-sulfur (Fe-S) clusters are essential cofactors for a wide range of metabolic enzymes, and their biosynthesis is tightly coordinated with cellular metabolic state. Cysteine desulfurases, such as NifS, initiate Fe-S cluster biogenesis by mobilizing sulfur from cysteine. We determined the crystal structures of *Azotobacter vinelandii* cysteine desulfurase NifS bound to the dicarboxylate metabolites malonate and succinate at near-atomic resolutions. Remarkably, both metabolites occupy the canonical substrate (cysteine) binding site and coordinate with Arg351 to sterically occlude substrate access. Enzymatic assays confirmed that malonate and succinate act as competitive inhibitors, reducing NifS activity by approximately 10% *in vitro*. Although the inhibitory effect is modest, these findings suggest a direct structural mechanism by which central carbon metabolites modulate the entry point of Fe-S cluster biosynthesis. We hypothesize that the accumulation of dicarboxylates under specific physiological conditions, such as high TCA cycle flux or redux imbalance, may act as a feedback signal to transiently attenuate Fe-S cluster formation. This study reveals a potential metabolic checkpoint linking Fe-S homeostasis to dicarboxylate metabolism and establishes a structural framework for exploring metabolite-mediated regulation of cofactor biosynthesis.

[PP-05]

Unveiling Photo-excited Electron Trapping Dynamics at Self-Reduced TiO_2 via Time-Resolved X-ray Absorption Spectroscopy

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Understanding the nonequilibrium photoexcited dynamics of photo-induced charge carriers in semiconducting photocatalysts is crucial for optimizing solar-to-chemical energy conversion. Titanium dioxide (TiO_2), owing to its photostability and tunable surface chemistry, serves as a prototypical system for such studies. However, TiO_2 has a limitation in absorbing visible energy, which occupies ~46% of the solar spectrum due to its relatively large bandgap energy (3.0-3.2 eV). To overcome this issue, we synthesized the self-reduced TiO_2 (blue TiO_2) to contain microstates as trap sites within the bandgap to enhance the visible light absorbance. In this study, we employed femtosecond time-resolved X-ray absorption spectroscopy (TRXAS) and nanosecond transient absorption spectroscopy (ns-TA) to elucidate the photo-induced charge carrier dynamics in both pristine and trap sites introduced TiO_2 nanoparticles. Steady-state X-ray absorption analysis confirmed the formation of Ti^{3+} species and defect-associated microstates, which modify the electronic structure and facilitate sub-bandgap absorption. TRXAS at the Ti K-edge revealed stronger pre-edge and edge transient signals in blue TiO_2, attributed to electron trapping at penta-coordinated Ti defect sites. Kinetic analysis showed similar ultrafast dynamics at the vicinity of the conduction band minimum in both materials, but also revealed that the shallow trap sites mediated decay pathway is the major relaxation process in blue TiO_2. The ns-TA measurements further confirmed long-lived charge separation in blue TiO_2, with excited-state absorption dominating over ground-state bleach. The understanding of the full dynamics of the photo-excited electron in the bare and oxygen vacancy-induced trap states introduced TiO_2 can play a key role in not only highlighting the potential of defect-rich TiO_2 for solar-driven photocatalysis but also designing the visible-light absorbing photocatalysts more efficiently.

[PP-06]

The correlation between crystal defect and plasma induced by femtosecond laser in crystalline Cu thin-films

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Understanding the interplay between lattice defects and laser-induced structural dynamics is essential to advance ultrafast material processing and energy conversion. Here, we report the microscale observation of femtosecond laser-induced ablation and shock wave generation in single crystalline Cu thin films using ultrafast time-resolved dark-field X-ray microscopy (DFXM) with hard X-rays with atomic resolution sensetivity. We successfully observed early stage of ablation at surface by showing Newtonring formation within picoseconds and tracks subsonic shock wave propagation along in-plane direction at nanosecond timescales. Crucially, we find that shock waves emerge exclusively in regions with some grain boundary density rather than no grain boundary, suggesting that crystallographic defects act as localized energy concentrators. Complementary experiments on TiO2 reveal that shock waves are observed only when the pump photon energy exceeds the band gap, highlighting the role of excited carrier generation. These findings establish defect-assisted energy localization as a key mechanism for initiating shock wave formation under ultrafast laser excitation, offering new strategies for tailoring laser-matter interaction through microstructural and electronic design.

[PP-07]

Crystallographic Snapshots of an ATP-bound Human p97 N-D1 Hexamer using X-ray Free-Electron Lasers

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The human ATPase p97, a member of the ATPases Associated with diverse cellular Activities (AAA+) superfamily, regulates numerous cellular pathways by unfolding a wide range of protein substrates. This ATP-dependent unfolding process is vital for maintaining protein homeostasis, making p97 a prominent therapeutic target. The hexameric p97 undergoes significant conformational changes during its catalytic cycle. In this study, we performed a crystallographic analysis of the p97 N-D1 hexamer using X-ray free-electron lasers (XFEL). Data were collected from microcrystals of the p97 N-D1 hexamer in the presence of excess adenosine triphosphate (ATP), yielding the first room-temperature structure of p97 in an ATP-bound-like state. Although the structure contains adenosine diphosphate (ADP), the key residues such as the arginine finger (Arg359) and Phe360 adopt conformations characteristic of the ATP-bound state. Additionally, the N-terminal domain exhibits a 4-degree rotation. Despite the relatively high R_{split} value and low resolution (3.5 Å), our results demonstrate that serial femtosecond crystallographic studies using XFEL can capture the intermediate states during ATP hydrolysis. Future high-resolution studies of ATP turnover in p97 will shed light on its intricate spatial and temporal regulation and support structure-based drug development.

[PP-08]

Void evolution in ultrafast melting of Au nanoparticles driven by light's angular momentum using time-resolved imaging at XFEL

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Ultrafast phase transitions in nanoscale systems can be directed by tailoring the angular momentum of light. In this study, we employ time-resolved single-particle imaging at an XFEL to investigate how the angular momentum state of light influences the melting dynamics of single Au nanoparticles. By comparing circularly polarized (Cir. pol.) and orbital angular momentum (OAM) excitation, we uncover distinct void formation pathways: under OAM excitation, voids nucleate directly at the nanoparticle center. In contrast, Cir. pol. excitation induces a vortex-like inward motion of the melting front, forming voids as the material spirals toward the center. This contrast suggests that photonic angular momentum reshapes the spatial patterns of energy deposition and stress evolution during melting. These findings highlight angular-momentum–dependent control of nonequilibrium phase transitions.

[PP-09]

Tracking Ligand Charge Delocalization Mediated Charge transfer dynamics of Bridged bimetallic complex

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Inspired by the process of photosynthesis, donor-bridge-acceptor systems have been proposed and studied. The electron transfer is mediated by the bridge between donor and acceptor. This bridge introduces electron correlation, which can have either beneficial or detrimental effects. The photoinduced charge transfer dynamics in the bridged bimetallic complex have been studied using transient absorption spectroscopy (TAS). However, the overlapping signals of excited states at each metal site are challenging to disentangle in TAS, hindering intuitive interpretation. Here, we employed atom specific femtosecond-resolved X-ray absorption spectroscopy (XAS) to investigate the charge-transfer dynamics of the bridged bimetallic Ru(II)-Os(II) complex ($[(bpy)_2Ru(tpphz)Os(bpy)_2]^{4+}$). The empty valence electronic state of the metal site is probed through the dipole-allowed $2p_{3/2}$ to empty valence d orbital transition. Due to the intense and temporally narrow X-ray pulse of PAL-XFEL, we can capture early dynamical features with relatively low amount of sample (1.5 mM concentration). The Metal-to-Ligand-Charge-Transfer (MLCT)-mediated electron transfer from Os to Ru was directly probed via the anticorrelation between the transient Os and Ru L_3-edge XAS spectra. Combined with theoretical calculations, the charge-localized and charge-delocalized MLCT states at the Os site were identified due to the significant coupling between the Os-N bonding structure and the ligand charge density, incontrast to MLCTs at the Ru site. Based on the density functional theory based ΔSCF calculation, the slight structural modulation in the Ru site caused by ligand charge delocalization increases the gap between MLCT(Ru) and MLCT(Os), enhancing charge transfer efficiency.

[PP-10]

Development of Femtosecond X-ray Emission Spectrometer Based on von Hamos geometry

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Recent advances in XFEL technology, particularly the generation of ultrashort X-ray pulses, have propelled the development of femtosecond X-ray spectroscopy using optical pump-X-ray probe techniques. Femtosecond X-ray absorption spectroscopy (fs-XAS) is pertinent to investigate the electronic structures and reaction dynamics of various chemical systems. In principle, it has a limitation to detect changes in electronic spin states. In this study, we aim to develop femtosecond X-ray emission spectroscopy (fs-XES) based on a von Hamos geometry. This approach leverages the ability of XES to probe valence orbitals and valence-to-core transitions, providing meaningful insights into spin-state dynamics at the atomic level. Our work focuses on fs-XES experiments conducted in the hard X-ray regime (5-12 keV) with the superb spectral resolution. The spectrometer configuration consists of 16 silicon crystal analyzers arranged in an array and a two-dimensional detector capable of single-photon detection. As a pilot experiment, we carried out fs-XES measurements targeting the Fe K_β emission line (7.06 keV) to observe photoinduced spin crossover dynamics in iron-based complexes. Our results suggest that the fs-XES will be a new experimental platform to study the electronic spin dynamics of metallic complexes in terms of orbital resolution.

[PP-11]

Evidence of a light-induced metastable state in charge-ordered 4*d*-kagome metals

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Kagome lattice materials can possess many competing charge order phases due to its frustrated geometry and intrinsic band singularities, which leads to potential metastable states in its free energy landscape. In this work, using time-resolved X-ray diffraction at PAL-XFEL, we investigated charge order dynamics of a newly discovered 4*d*-kagome metal $LuNb_6Sn_6$. The dynamics in $LuNb_6Sn_6$ are characterized by ultrafast melting within 300 fs followed by the launch of coherent amplitude mode oscillation, a typical signature of phonon-coupled charge order state. The amplitudon frequency of $LuNb_6Sn_6$ was found to be 1.2 THz, slower than that of the 3*d*-kagome counterpart ScV_6Sn_6. Notably, our single-shot experiment reveals that the charge order amplitude remain suppressed for substantial timescales, more than a few seconds, evidencing a potential light-induced transition to metastable states. The nature of metstable states in $LuNb_6Sn_6$ remains unknown at this stage and will be a subject of subsequent studies.